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Single-Crystal Structure of HP-Sc₂TeO₆ Prepared by High-Pressure/High-Temperature Synthesis

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Abstract: The first high-pressure scandium tellurate HP-Sc₂TeO₆ was synthesized from an NP-Sc₂TeO₆ normal-pressure precursor at 12 GPa and 1173 K using a multianvil apparatus (1000 t press, Walker-type module). The compound crystallizes in the monoclinic space group *P2/c* (no. 13) with *a* = 729.43(3), *b* = 512.52(2), *c* = 1095.02(4) pm and $\beta = 103.88(1)^\circ$. The structure was refined from X-ray single-crystal diffractometer data: *R*₁ = 0.0261, *wR*₂ = 0.0344, 568 *F*² values and 84 variables. HP-Sc₂TeO₆ is isostructural to Yb₂WO₆ and is built up from TeO₆ octahedra, typical for tellurate(VI) compounds. During synthesis, a reconstructive transition from *P321* (normal-pressure modification) to *P2/c* (high-pressure modification) takes place and the scandium–oxygen distances as well as the coordination number of scandium increase. However, the coordination sphere around the Te⁶⁺ cations gets only slightly distorted. High-temperature powder XRD investigations revealed a back-transformation of HP-Sc₂TeO₆ to the ambient-pressure modification above 973 K.

Keywords: high-pressure; crystal structure; scandium tellurate; tellurate(VI)

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1. Introduction

Transition metal tellurates show a broad variety of technologically important properties. M₃TeO₆ (M = Ni, Co, Mn, Cu) compounds exhibit antiferromagnetic ordering at low temperatures combined with magnetoelectric properties. These materials are classified as type-II multiferroics and have recently gained great importance [1–8]. The structural diversity of oxotellurate compounds is related on Te⁴⁺ and Te⁶⁺ as well as mixed valent Te⁴⁺/Te⁶⁺ combinations. Oxotellurate(IV) anions are characterized by the presence of the 5s² lone-electron pair, which causes various oxygen coordination spheres with coordination numbers from three to five and a wide range of possible Te–O bond-lengths. Moreover, stereoactive lone-pair electrons and their directing effects on the crystal structure are responsible for the excellent SHG efficiencies of tellurate crystals [9,10].

Scandium forms both oxotellurates(IV) and oxotellurates(VI), and a total of only three compounds, have been fully described so far. Sc₂Te₅O₁₃ and Sc₂Te₃O₉ are oxotellurate(IV) representatives. The crystal structure of Sc₂Te₅O₁₃ [11] is triclinic with space group *P* $\bar{1}$ (no. 2) and isopuntal to Lu₂Te₅O₁₃ [12]. In contrast to Sc³⁺, all other compounds with the formula type M₂Te₅O₁₃ (M = Y, Dy–Lu) exhibit significantly larger coordination spheres at the M³⁺ sites [11–13]. The second compound, Sc₂Te₃O₉, crystallizes monoclinic (*P2*₁/*n*, no. 14) and is built up from ScO₆ octahedra, ScO₇-capped octahedra and TeO₃ trigonal pyramids [14]. Additional representatives of the composition M₂Te₃O₉ (M = Ga, In, Dy and Lu) form different crystal structure types [15–17]. Two additional Sc–Te–O phases published without structural details can be found in the PDF4+ 2021 [18] database, i.e., Sc₆TeO₁₂ (PDF# 04-002-9406, [19]) and Sc₂Te₄O₁₁ (PDF# 00-047-0010).

In oxotellurate(VI) chemistry, the general formula M₂TeO₆ is common. Three crystal structure types are mainly prevalent: the Na₂SiF₆-type structure, which crystallizes trigonal

in the space group $P321$ (no. 150) and the two orthorhombic structure types Ta_2FeO_6 ($P4_2/mnm$, no. 136) and Nd_2WO_6 ($P2_12_12_1$, no. 19).

Recently, we focused our work on tellurate compounds at extreme conditions and were able to add now a fourth structure type to the M_2TeO_6 -system. To distinguish the new compound $\text{HP-Sc}_2\text{TeO}_6$ synthesized under high-pressure (HP), the phase synthesized under normal-pressure (NP) will be referred to as $\text{NP-Sc}_2\text{TeO}_6$ [11] in the following. Here we present the synthesis, crystal structure and high-temperature behaviour of $\text{HP-Sc}_2\text{TeO}_6$.

2. Materials and Methods

$\text{HP-Sc}_2\text{TeO}_6$ was synthesized via high-pressure/high-temperature multianvil experiments according to Equation (1). $\text{NP-Sc}_2\text{TeO}_6$ served as precursor and was prepared through a high-temperature solid state route from Sc_2O_3 (powder, purity 99.99%, ChemPUR, Karlsruhe, Germany) and TeO_3 in a 1:1 ratio under air.

To obtain $\text{NP-Sc}_2\text{TeO}_6$, a homogeneous mixture of the reagents was filled in a corundum boat and heated to 1073 K within 6 h. The temperature was kept constant for 36 h. TeO_3 was synthesized by dehydration of $\text{Te}(\text{OH})_6$ (powder, purity > 99.0%, TCI, Tokyo, Japan) in a corundum boat at 623 K for 36 h in air.

For the high-pressure/high-temperature transformation to $\text{HP-Sc}_2\text{TeO}_6$, the precursor $\text{NP-Sc}_2\text{TeO}_6$ was homogenised and filled in a platinum capsule. The capsule was placed in a crucible made of hexagonal boron nitride and covered by a platelet of the same material (Henze Boron Nitride Products AG, Kempten, Germany). Together with two graphite sleeves acting as resistive heaters, a ZrO_2 sleeve for temperature isolation and two molybdenum platelets to ensure conductivity, the crucible was centred in an octahedron of MgO doped with 5% Cr_2O_3 as the pressure medium. The compression of the specimen was accomplished by a two-stage mechanism of eight inner anvils (first stage) consisting of tungsten carbide cubes with truncated corners (Hawedia, Marklkofen, Germany) and centred octahedral pressure medium. The second stage, the Walker-type module of the 1000 t uniaxial press (both devices from Max Voggenreiter GmbH, Mainleus, Germany), houses the inner anvils with the sample. Detailed information about the multianvil technique and the construction of the various assemblies can be found in numerous references [20–23].

The pressure was ramped up to 12 GPa in 320 min followed by heating the sample to 1173 K within 10 min. This temperature was kept for the next 10 min and then reduced to 673 K within 20 min. A temperature quench to room temperature completed the heating period and subsequently the pressure was reduced to ambient conditions in 1000 min. Afterwards, the sample was recovered by removing the surrounding assembly materials through mechanical fragmentation. The sample appeared colourless, polycrystalline and was stable at air.

X-ray powder diffraction experiments were conducted on a STOE STADI P diffractometer (STOE & Cie GmbH, Darmstadt, Germany) with (111) curved Ge-monochromatized $\text{Mo-K}_{\alpha 1}$ radiation ($\lambda = 70.93$ pm) in transmission geometry. The diffraction intensities were collected by a DECTRIS MYTHEN 1K microstrip detector with 1280 strips. Polycrystalline samples of $\text{HP-Sc}_2\text{TeO}_6$ were ground in an agate mortar and placed between two thin acetate foils.

Rietveld refinement was accomplished with the software package DIFFRAC^{plus}-TOPAS 4.2 (Bruker AXS, Karlsruhe, Germany). The refinement was based on the single-crystal structure model and the peak shapes were optimized using modified Thompson–Cox–Hastings pseudo-Voigt profiles [24,25]. The lattice parameters derived from the refinement are comparable with those received by single-crystal X-ray diffraction (see Table 1). Moreover, theoretical powder pattern calculated from the single-crystal data fits well to the measured powder pattern, which proves the purity of the $\text{HP-Sc}_2\text{TeO}_6$ specimen (see Figure 1).

Table 1. Crystal data, data collection and structure refinement results for HP-Sc₂TeO₆.

Empirical formula	HP-Sc ₂ TeO ₆
Molar mass, g·mol ^{−1}	313.52
Crystal system	monoclinic
Space group	<i>P2₁/c</i>
Cell formula units	4
Powder diffractometer	STOE STADI P
Radiation	Mo-K _{α1} (λ = 70.93 pm)
Powder data:	
<i>a</i> , pm	729.224(7)
<i>b</i> , pm	512.576(5)
<i>c</i> , pm	1095.04(2)
β, deg	103.898(1)
<i>V</i> , Å ³	397.323(7)
Single-crystal diffractometer	Bruker D8 Quest
Radiation	Mo-K _α (λ = 71.073 pm)
Single-crystal data:	
<i>a</i> , pm	729.43(3)
<i>b</i> , pm	512.52(2)
<i>c</i> , pm	1095.02(4)
β, deg	103.88(1)
<i>V</i> , Å ³	397.42(3)
Calculated density, g·cm ^{−3}	5.24
Crystal size, mm ³	0.02 × 0.02 × 0.02
Temperature, K	299(2)
Absorption coefficient, mm ^{−1}	10.54
<i>F</i> (000), <i>e</i>	568
Detector distance, mm	34
θ range, deg	2.88–39.42
Range in <i>hkl</i>	−12 ≤ <i>h</i> ≤ 13, ±9, ±19
Total no. reflections	13924
Data/ref. parameters	2379/84
Reflections with <i>I</i> > 2σ(<i>I</i>)	2077
<i>R</i> _{int} / <i>R</i> _σ	0.0363, 0.0254
Goodness-of-fit on <i>F</i> ²	1.055
Absorption correction	multi-scan
<i>R</i> ₁ / <i>wR</i> ₂ for <i>I</i> > 2σ(<i>I</i>)	0.0191/0.0331
<i>R</i> ₁ / <i>wR</i> ₂ for all data	0.0261/0.0344
Extinction coefficient	0.0026(2)
Transmission max./min.	0.748/0.646
Largest diff. peak/hole/ <i>e</i> ·Å ^{−3}	0.905/−0.962

Figure 1. XRPD pattern (Mo-K_{α1} radiation) and Rietveld refinement of X-ray pure HP-Sc₂TeO₆ displayed with an offset of 750 counts (*R*_{exp} = 6.98, *R*_{wp} = 7.56, *R*_p = 5.67 and *Goof* = 1.08).

A single-crystal was isolated in perfluoropolyalkylether (viscosity 1800 cSt) and mounted on the tip of a loop (MicroMountsTM, MiTeGen, LLC, Ithaca, NY, USA) using a microscope. The data collection was conducted at a Bruker D8 Quest diffractometer (Bruker AXS, Karlsruhe, Germany) equipped with an Incoatec IμS sealed tube microfocus source with multi-layered optic producing monochromatized Mo-K_α radiation (λ = 71.073 pm) and a Photon 100 CMOS detector. The diffraction patterns were indexed and the total number of runs and images was based on the strategy calculation from the program APEX3 [26].

The unit cell refinement, integration and data reduction were performed using SAINT [26]. A semi-empirical multi-scan absorption correction was carried out using SADABS [26].

X-ray powder diffraction patterns at elevated temperatures were recorded using a Rigaku SmartLab-3kW instrument in parallel beam setting and reflection mode ($\text{Cu-K}\alpha$, $\lambda = 154.18$ pm) using a HyPix3000 detector (Rigaku, Tokyo, Japan). The ground sample was placed on a flat Al_2O_3 -sample holder compatible with an Anton Paar HTK1200N (Anton Paar, Graz, Austria) high-temperature chamber used for heating. The patterns were recorded in a range of 15 to $60^\circ 2\theta$ with a step width of 0.01° and a speed of $1.5^\circ/\text{min}$. The temperature was increased by 20 K/min and held for one minute before each measurement. Patterns were recorded in 100 K steps up to 773 K and subsequently in 50 K steps up to 1373 K, on temperature decrease, a measurement was performed every 100 K.

SmartLab Studio-II (Rigaku Corporation 2014) was used for data collection, temperature control and data analysis such as phase identification and WPPF refinement. For phase identification, the PDF4+ 2021 [18] database was used.

Semiquantitative analyses by energy-dispersive X-ray spectroscopy (EDX) on several crystals of $\text{HP-Sc}_2\text{TeO}_6$ were made using a scanning electron microscope (JSM-6010LV, Jeol, Freising, Germany) with an energy-dispersive Quantax X-ray detector-system (Bruker AXS GmbH, Billerica, MA, USA) for element identification. The crystals were placed on a carbon plate on an aluminium sample carrier and sputtered with carbon. Each region was measured for 60 s at an excitation energy of 15 kV in high vacuum. Three crystals (see Figure 2) were measured regarding their Sc to Te ratio, and the values from several measurement points were arithmetically averaged. Due to the preparation method and the low sensitivity of light atoms like oxygen only, the ratio of scandium to tellurium was considered and the absolute values are neglected. The measured ratio of $\text{Sc/Te} = 36 \pm 3$ at% Sc/ 18 ± 3 at% Te agrees well with the theoretical ratio of $\text{Sc/Te} = 2:1$ in $\text{HP-Sc}_2\text{TeO}_6$.

Figure 2. Crystals of $\text{HP-Sc}_2\text{TeO}_6$ selected for elemental analysis by energy-dispersive X-ray spectroscopy (EDX).

3. Results and Discussion

3.1. Structure Refinements

$\text{HP-Sc}_2\text{TeO}_6$ crystallizes monoclinic with the following lattice parameters: $a = 729.43(3)$, $b = 512.52(2)$, $c = 1095.02(4)$ pm and $\beta = 103.88(1)^\circ$. The space group $P2_1/c$ (no. 13) was indicated by the general systematic extinctions of $h0l$ with $l \neq 2n$ and $00l$ with $l \neq 2n$ as well as the special extinction conditions hkl : $l \neq 2n$. Using the “Intrinsic Phasing” algorithm implemented in the APEX3 program package [27], the initial positional parameters were determined. Full-matrix least-squares refinements based on F^2 yielded the exact atom posi-

tions [28,29] and finally, all atoms were refined with anisotropic displacement parameters. The occupation parameters were refined in a separate series of least-squares cycles in order to verify the correct composition. The correctness of the space group was proved with the ADDSYM [30] routine of the PLATON program package [31]. Experimental details, the positional parameters and anisotropic displacement parameters are listed in Tables 1–3. CSD 2124916 (HP-Sc₂TeO₆) contains the ESI data for this paper.

Table 2. Atomic coordinates, Wyckoff positions, site occupancy (s. o. f.) and equivalent isotropic displacement parameters U_{eq} (Å²)¹ for HP-Sc₂TeO₆ (space group *P2/c*; no. 13). Standard deviations in parentheses.

Atom	Wyck.	<i>x</i>	<i>y</i>	<i>z</i>	SOF	U_{eq}
Te1	4g	0.22848(2)	0.26270(2)	0.61484(2)	1	0.00223(3)
Sc1	4g	0.71575(4)	0.19306(6)	0.58249(3)	1	0.00365(5)
Sc2	2f	1/2	0.24868(8)	1/4	1	0.00377(6)
Sc3	2e	0	0.30665(8)	1/4	1	0.00442(7)
O1	4g	0.0135(2)	0.6152(2)	0.3823(2)	1	0.0050(2)
O2	4g	0.1418(2)	0.1363(2)	0.4484(1)	1	0.0056(2)
O3	4g	0.2041(2)	0.0254(2)	0.2271(1)	1	0.0044(2)
O4	4g	0.3021(2)	0.5402(2)	0.2758(1)	1	0.0046(2)
O5	4g	0.3462(2)	0.4355(2)	0.0674(1)	1	0.0054(2)
O6	4g	0.4541(2)	0.0606(2)	0.6107(2)	1	0.0050(2)

¹ U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters U_{ij} (Å²)¹ for HP-Sc₂TeO₆ (space group *P2/c*; no. 13). Standard deviations in parentheses.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te1	0.00242(4)	0.00213(4)	0.00227(4)	−0.00001(3)	0.00082(3)	0.00006(3)
Sc1	0.0040(1)	0.0037(1)	0.0036(1)	0.00032(8)	0.00160(8)	0.00024(8)
Sc2	0.0041(1)	0.0030(2)	0.0041(1)	0	0.0006(1)	0
Sc3	0.0047(2)	0.0034(2)	0.0055(2)	0	0.0019(1)	0
O1	0.0031(4)	0.0062(5)	0.0060(4)	−0.0009(4)	0.0017(4)	0.0006(4)
O2	0.0076(5)	0.0054(5)	0.0030(4)	−0.0018(3)	−0.0004(4)	0.0007(4)
O3	0.0059(4)	0.0031(4)	0.0043(4)	−0.0013(3)	0.0013(4)	0.0006(4)
O4	0.0068(5)	0.0043(4)	0.0027(4)	0.0010(3)	0.0012(4)	0.0017(4)
O5	0.0061(5)	0.0049(5)	0.0051(4)	−0.0013(4)	0.0010(4)	0.0015(4)
O6	0.0029(4)	0.0044(5)	0.0081(5)	0.0013(4)	0.0023(4)	0.0014(3)

¹ The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}]$.

3.2. Crystal Chemistry

HP-Sc₂TeO₆ forms at high-pressure/high-temperature conditions of 12 GPa and 1173 K from the normal-pressure precursor compound. It crystallizes in the monoclinic space group *P2/c* (no. 13) and is isostructural to Yb₂WO₆ [32]. The Te⁶⁺ cations are distorted octahedrally coordinated by six oxygen ions, whereas Sc1 is coordinated by seven oxygen ions as a capped trigonal prism. Sc2- and Sc3-atoms are distorted quadratic antiprismatically coordinated by eight oxygen ions. All coordination geometries with given atom distances are displayed in Figure 3.

Figure 3. Coordination spheres and interatomic distances (pm) of Te1 (top left), Sc1 (top right), Sc2 and Sc3 (bottom left and right). Standard deviations are smaller than 0.2 pm.

The crystal structure is built up by two alternating layers A and B (Figure 4, top). In layer A, square antiprisms of Sc_2O_8 share edges with four octahedra of TeO_6 , which in turn are connected to two Sc_2O_8 units. Thus, the polyhedra form unconnected bands along the crystallographic b -axis. Layer B consists of Sc_3O_8 and Sc_1O_7 units, which are similarly connected to each other as in layer A. The resulting bands are edge connected via the Sc_1O_7 polyhedra, unlike in layer A. Both layers are linked via corners and edges stacked along $[10\bar{1}]$ (Figure 4, bottom). The Te–O distances vary between 188.0 and 199.0 pm, which is in good agreement with other tellurates(VI) [33]. The fourfold linked oxygen atom O4 exhibits the longest Te–O distance. The Sc–O distances in HP- Sc_2TeO_6 are longer than in Sc_2O_3 (208 to 216 pm), which agrees well with the pressure coordination rule [34,35]. A comparison with the normal-pressure modification NP- Sc_2TeO_6 is given later on in the section. Sc1 has six shorter (202.1 to 231.5 pm) and one longer (253.8 pm) distance to oxygen atoms. The long distance between Sc1 and O6 is responsible for the connection of the bands in layer B. The quadratic antiprismatically coordinated atoms Sc2 and Sc3 show similar distances to oxygen atoms of 214.3 to 240.2 pm and 213.0 to 246.4 pm, respectively.

NP- Sc_2TeO_6 [11] crystallizes in the Na_2SiF_6 -type structure (trigonal, $P321$, no. 150). The structural differences between the high-pressure and normal-pressure modifications of Sc_2TeO_6 are confirmed by changes in molar volume, coordination numbers and atom distances. The molar volume decreases from the normal-pressure phase to the high-pressure phase from $63.73 \text{ cm}^3 \cdot \text{mol}^{-1}$ to $59.83 \text{ cm}^3 \cdot \text{mol}^{-1}$. The coordination of tellurium remains unchanged, but the distortion is enhanced in the high-pressure phase. On the one hand, this is indicated by different Te–O distances; on the other hand, the distortion is seen in the angles of the octahedra. The axial octahedra angles range from 154° to 169° (ideal: 180°) and the equatorial angles from 78° to 107° (ideal: 90°). In any case, the average Te–O distances do not change significantly between the normal-pressure (191 pm) and high-pressure (193 pm) modifications. In contrast to the coordination of the Te atoms, the coordination number of all three scandium atoms increases from six in the normal-pressure modification to seven and eight in the high-pressure phase. Therefore, Sc–O distances increase from NP- Sc_2TeO_6 (208.4 to 216.4 pm) to HP- Sc_2TeO_6 (202.2 to 253.8 pm), with most distances longer than 208 pm.

Figure 4. The crystal structure of HP-Sc₂TeO₆ is shown with view along the *b* axis (bottom). Layer (A) (top left) and layer (B) (top right) are displayed along the crystallographic *c* axis.

3.3. Theoretical Calculations

For better evidence of the crystal structure of HP-Sc₂TeO₆ MAPLE (Madelung Part of Lattice Energy), CHARDI (Charge Distribution) as well as BL/BS (bond length/bond strength) calculations have been performed [36–41]. The calculated bond-valence sums and charge distributions agree well with the formal charges Te⁶⁺, Sc³⁺ and O^{2−} acquired by X-ray structure analysis (see Table 4).

Table 4. Charge distribution calculated with BL/BS (ΣV) and CHARDI (ΣQ).

	Te1	Sc1	Sc2	Sc3	O1	O2	O3	O4	O5	O6
ΣV	+5.83	+3.08	+2.86	+2.78	−2.01	−1.91	−1.72	−1.98	−2.00	−1.96
ΣQ	+5.99	+2.99	+3.03	+3.01	−2.12	−1.98	−1.89	−1.99	−2.08	−1.93

The MAPLE_{ter} value of HP-Sc₂TeO₆ (42,018 kJ/mol) fits to the MAPLE_{bin} value (42,159 kJ/mol) with a deviation of 0.3% or 141 kJ/mol, which is within the limits of the concept. MAPLE_{bin} is calculated by the sum of MAPLE_{Sc2O3} (16,435 kJ/mol) and MAPLE_{TeO3} (25,724 kJ/mol) in stoichiometric ratio.

3.4. Temperature-Dependent X-ray Powder Diffractometry

To investigate the high-temperature behaviour of HP-Sc₂TeO₆, temperature-dependent X-ray powder diffractometry was performed (see Figure 5). At the starting temperature of 298 K, all measured Bragg reflections could be indexed with HP-Sc₂TeO₆ and sample holder material Al₂O₃. In comparison to the X-ray powder diffraction experiments performed in transmission geometry (see Figure 1), the patterns recorded in reflection geometry showed a strong preferred orientation for (10 $\bar{2}$), presumably due to the sample preparation. At 298 K, the lattice parameters of HP-Sc₂TeO₆ were determined as *a* = 728.89(3), *b* = 512.11(2), *c* = 1094.67(4) pm, β = 103.95(2)°. With increasing temperature lattice parameters expanded to *a* = 731.9(1), *b* = 514.39(7), *c* = 1105.7(1) pm, β = 103.28(2)° at 1073 K. Bragg reflections

of HP-Sc₂TeO₆ decreased in intensity at 1073 K, were still present at 1123 K but absent at 1173 K. At 973 K, Bragg reflections of a new phase appeared with very little intensity and increased in intensity at 1123 K. They dominated the pattern from 1123 to 1223 K and decreased at 1273 K, at 1323 K they were not observed any more. This phase, observed overall from 973 to 1273 K, has been identified as NP-Sc₂TeO₆ [11]. However, whole powder pattern fitting did not yield satisfying results due to very different peak shapes: some Bragg reflections, especially (101), (201), (211) and some further reflections of lower intensity, were significantly broadened compared to (110), (111), (300) and (302). The reason for this could be (1) the formation of an unidentified HT-phase overlapping with NP-Sc₂TeO₆ or (2) anisotropic peak broadening of NP-Sc₂TeO₆ due to crystal shape anisotropy.

Figure 5. Temperature-dependent X-ray powder diffractogram displaying the back-transformation of HP-Sc₂TeO₆ to the ambient pressure modification NP-Sc₂TeO₆.

Another phase started to appear from at least 1123 K, it was identified as Sc₆TeO₁₂, $R\bar{3}$ isostructural to Y₂UO₁₂ [18,19]. Besides signals from the Al₂O₃ sample holder, Sc₆TeO₁₂ was the only phase present at 1323 and 1373 K and remained stable on temperature decrease to 298 K. Lattice parameters were determined as $a = 933.53(2)$, $c = 884.31(5)$ pm at 1373 K and $a = 924.47(2)$, $c = 873.40(2)$ pm at 298 K.

4. Conclusions

The structural elucidation of the first scandium tellurate (HP-Sc₂TeO₆) synthesized under high-pressure/high-temperature conditions of 12 GPa and 1173 K revealed a Yb₂WO₆-type structure. The normal-pressure modification of Sc₂TeO₆ adopts the Na₂SiF₆-type structure. From a crystal symmetry point of view, there exists no direct group subgroup relationship between the two space groups $P321$ and $P2/c$. Thus, a reconstructive conversion of the precursor material NP-Sc₂TeO₆ to HP-Sc₂TeO₆ can be assumed. High-temperature powder X-ray diffractometry characterized the back-transformation of the metastable high-pressure modification to the at ambient conditions thermodynamically stable NP-Sc₂TeO₆ modification. Rietveld refinements confirmed the single-crystal structure model and the purity of the product.

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